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4. The method of claim 1, wherein said ligand comprises a nicotinamide adenine dinucleotide-related molecule.

5. The method of claim 4, wherein said
5 nicotinamide adenine dinucleotide-related molecule is selected from the group consisting of oxidized nicotinamide adenine dinucleotide, reduced nicotinamide adenine dinucleotide, oxidized nicotinamide adenine dinucleotide phosphate, reduced nicotinamide adenine dinucleotide
10-phosphate, and a mimetic thereof.

6. A method for identifying a member of a pharmacocluster, comprising:

(a) determining a bound conformation of a ligand bound to a polypeptide; and

15 (b) determining a pharmacocluster having substantially the same bound conformation as said bound conformation, thereby identifying said bound conformation of said ligand as a member of said pharmacocluster.

7. The method of claim 6, wherein substantially
20 the same bound conformation comprises a root mean square deviation of less than 1.1 Å.

8. The method of claim 6, wherein said ligand is selected from the group consisting of adenosine triphosphate, adenosine diphosphate, adenosine monophosphate thiamine (vitamin B₁), riboflavin (vitamin B₂), pyridoximine
5 (vitamin B₆), cobalamin (vitamin B₁₂), pyrophosphate, flavin adenine dinucleotide (FAD), flavin mononucleotide (FMN), pyridoxal phosphate, coenzyme A, ascorbate (vitamin C), niacin, biotin, heme, porphyrin, folate, tetrahydrofolate, guanosine triphosphate, cytidine triphosphate, thymidine
10 triphosphate, uridine triphosphate, retinol (vitamin A), calciferol (vitamin D₂), ubiquinone, ubiquitin, α -tocopherol (vitamin E), farnesyl, geranylgeranyl, pterin, pteridine or S-adenosyl methionine (SAM).

9. The method of claim 6, wherein said ligand
15 comprises a nicotinamide adenine dinucleotide-related molecule.

10. The method of claim 9, wherein said
nicotinamide adenine dinucleotide-related molecule is selected from the group consisting of oxidized nicotinamide
20 adenine dinucleotide, reduced nicotinamide adenine dinucleotide, oxidized nicotinamide adenine dinucleotide phosphate, reduced nicotinamide adenine dinucleotide phosphate, and a mimetic thereof.

11. A method for identifying a conformation-dependent property of a ligand, comprising:

(a) determining bound conformations of a ligand bound to different polypeptides;

5 (b) identifying two or more bound conformations of said ligand having substantially the same bound conformation; and

(c) identifying a conformation-dependent property of said bound conformations of said ligand having
10 substantially the same bound conformation, said conformation-dependent property being correlated with said bound conformation of said ligand.

12. The method of claim 11, wherein said conformation-dependent property comprises a spectroscopic
15 signal.

13. The method of claim 11, wherein said conformation-dependent property comprises an NMR signal.

14. The method of claim 13, wherein said NMR signal is selected from the group consisting of chemical
20 shift, *J* coupling, dipolar coupling, cross-correlation, nuclear spin relaxation, transferred nuclear Overhauser effect, and any combination thereof.

15. The method of claim 11, wherein substantially the same bound conformation comprises a root mean square
25 deviation of less than 1.1 Å.

16. The method of claim 11, wherein said ligand is selected from the group consisting of adenosine triphosphate, adenosine diphosphate, adenosine monophosphate thiamine (vitamin B₁), riboflavin (vitamin B₂), pyridoximine
5 (vitamin B₆), cobalamin (vitamin B₁₂), pyrophosphate, flavin adenine dinucleotide (FAD), flavin mononucleotide (FMN), pyridoxal phosphate, coenzyme A, ascorbate (vitamin C), niacin, biotin, heme, porphyrin, folate, tetrahydrofolate, guanosine triphosphate, cytidine triphosphate, thymidine
10 triphosphate, uridine triphosphate, retinol (vitamin A), calciferol (vitamin D₂), ubiquinone, ubiquitin, α -tocopherol (vitamin E), farnesyl, geranylgeranyl, pterin, pteridine or S-adenosyl methionine (SAM).

15 17. The method of claim 11, wherein said ligand comprises a nicotinamide adenine dinucleotide-related molecule.

18. The method of claim 17, wherein said nicotinamide adenine dinucleotide-related molecule is
20 selected from the group consisting of oxidized nicotinamide adenine dinucleotide, reduced nicotinamide adenine dinucleotide, oxidized nicotinamide adenine dinucleotide phosphate, reduced nicotinamide adenine dinucleotide phosphate, and a mimetic thereof.

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(a) determining bound conformations of a ligand bound to different polypeptides of a polypeptide family; and

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21. The method of claim 19, wherein said ligand is selected from the group consisting of adenosine triphosphate, adenosine diphosphate, adenosine monophosphate thiamine (vitamin B₁), riboflavin (vitamin B₂), pyridoximine
5 (vitamin B₆), cobalamin (vitamin B₁₂), pyrophosphate, flavin adenine dinucleotide (FAD), flavin mononucleotide (FMN), pyridoxal phosphate, coenzyme A, ascorbate (vitamin C), niacin, biotin, heme, porphyrin, folate, tetrahydrofolate, guanosine triphosphate, cytidine triphosphate, thymidine
10 triphosphate, uridine triphosphate, retinol (vitamin A), calciferol (vitamin D₂), ubiquinone, ubiquitin, α -tocopherol (vitamin E), farnesyl, geranylgeranyl, pterin, pteridine or S-adenosyl methionine (SAM).

22. The method of claim 19, wherein said ligand
15 comprises a nicotinamide adenine dinucleotide-related molecule.

23. The method of claim 22, wherein said
nicotinamide adenine dinucleotide-related molecule is selected from the group consisting of oxidized nicotinamide
20 adenine dinucleotide, reduced nicotinamide adenine dinucleotide, oxidized nicotinamide adenine dinucleotide phosphate, reduced nicotinamide adenine dinucleotide phosphate, and a mimetic thereof.

(a) determining a conformation-dependent property of a ligand bound to a polypeptide; and

25. The method of claim 24, wherein said conformation-dependent property comprises a spectroscopic signal.

27. The method of claim 26, wherein said NMR signal is selected from the group consisting of chemical shift, *J* coupling, dipolar coupling, cross-correlation, nuclear spin relaxation, transferred nuclear Overhauser effect, and any combination thereof.

29. The method of claim 24, wherein said ligand is
15 a nicotinamide adenine dinucleotide-related molecule.

31. The method of claim 24, wherein said ligand is a adenosine phosphate-related molecule.

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42. A ligand conformer model, comprising a ligand conformer model, selected from the group consisting of conformer model 1 having coordinates listed in Table 3C, conformer model 2 having coordinates listed in Table 4C, 5 conformer model 3 having coordinates listed in Table 5C, conformer model 4 having coordinates listed in Table 6C, conformer model 5 having coordinates listed in Table 7C, conformer model 6 having coordinates listed in Table 8C, conformer model 7 having coordinates listed in Table 9C, and 10 conformer model 8 having coordinates listed in Table 10C.

43. A moiety, comprising coordinates, selected from the group consisting of coordinates listed in Table 3C, coordinates listed in Table 4C, coordinates listed in Table 5C, coordinates listed in Table 6C, coordinates listed in 15 Table 7C, coordinates listed in Table 8C, coordinates listed in Table 9C, and coordinates listed in Table 10C.

44. A pharmacophore model, comprising a pharmacophore model selected from the group consisting of pharmacophore model 1 having coordinates listed in Tables 3B 20 and 3C, pharmacophore model 2 having coordinates listed in Tables 4B and 4C, pharmacophore model 3 having coordinates listed in Tables 5B and 5C, pharmacophore model 4 having coordinates listed in Tables 6B and 6C, pharmacophore model 5 having coordinates listed in Tables 7B and 7C, 25 pharmacophore model 6 having coordinates listed in Tables 8B and 8C, pharmacophore model 7 having coordinates listed in Tables 9B and 9C, and pharmacophore model 8 having coordinates listed in Tables 10B and 10C.